OPTION A: ANALYTICAL CHEM A2 – PRINCIPLES OF SPECTROSCOPY

IB Chemistry

TAD01

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A2 – Principles of Spectroscopy

- A.2.1 Describe the electromagnetic spectrum. (2) *X-ray, ultraviolet (UV), visible, infrared (IR), radio and microwave should be identified. Highlight the variation in wavelength, wave number, frequency and energy across the spectrum.*
- A.2.2 Distinguish between absorption and emission spectra and how each is produced. (2)
- A.2.3 Describe the atomic and molecular processes in which absorption of energy takes place. (2) *The description should include vibrations, rotation an electronic transitions.*

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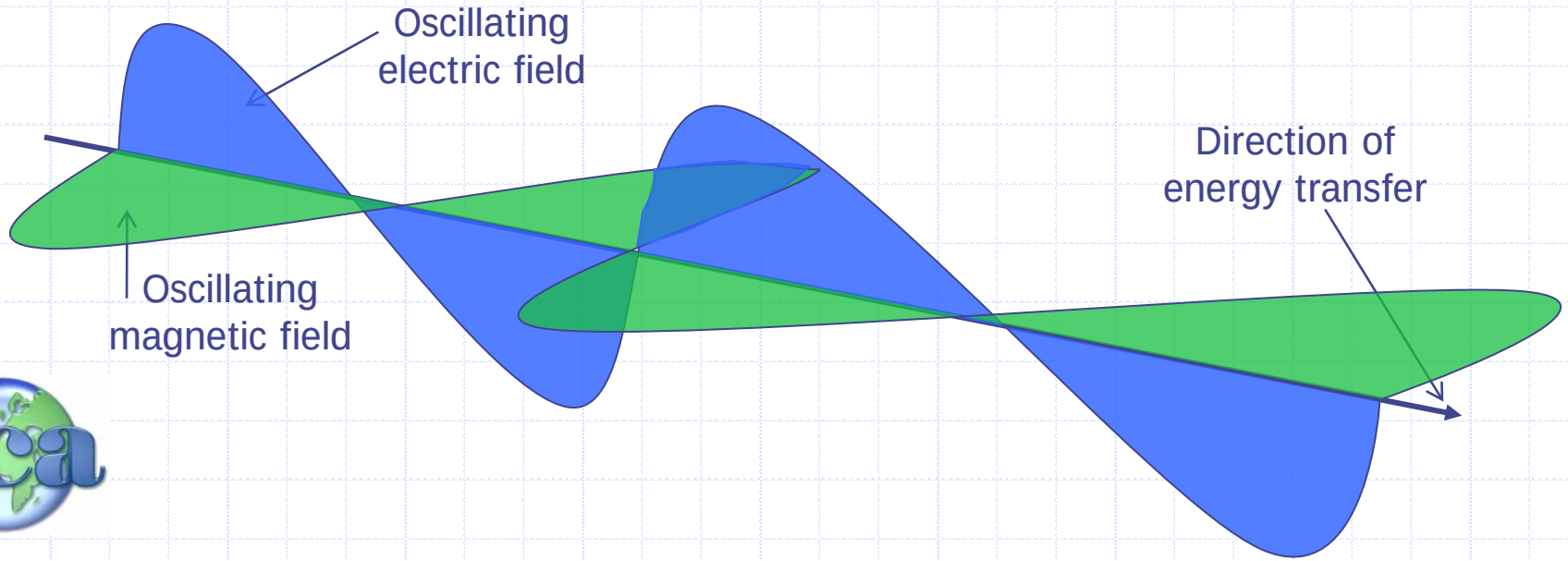
Electromagnetic Spectrum

A.2.1 Describe the electromagnetic spectrum. (2)

- Light is transformed in the form of **electromagnetic waves**
  - **Transverse waves** and can be polarized
  - These waves consist of oscillating **electric** and **magnetic** waves traveling together in a sinusoidal (sin) wave
  - They are **perpendicular** to one another (right angles)



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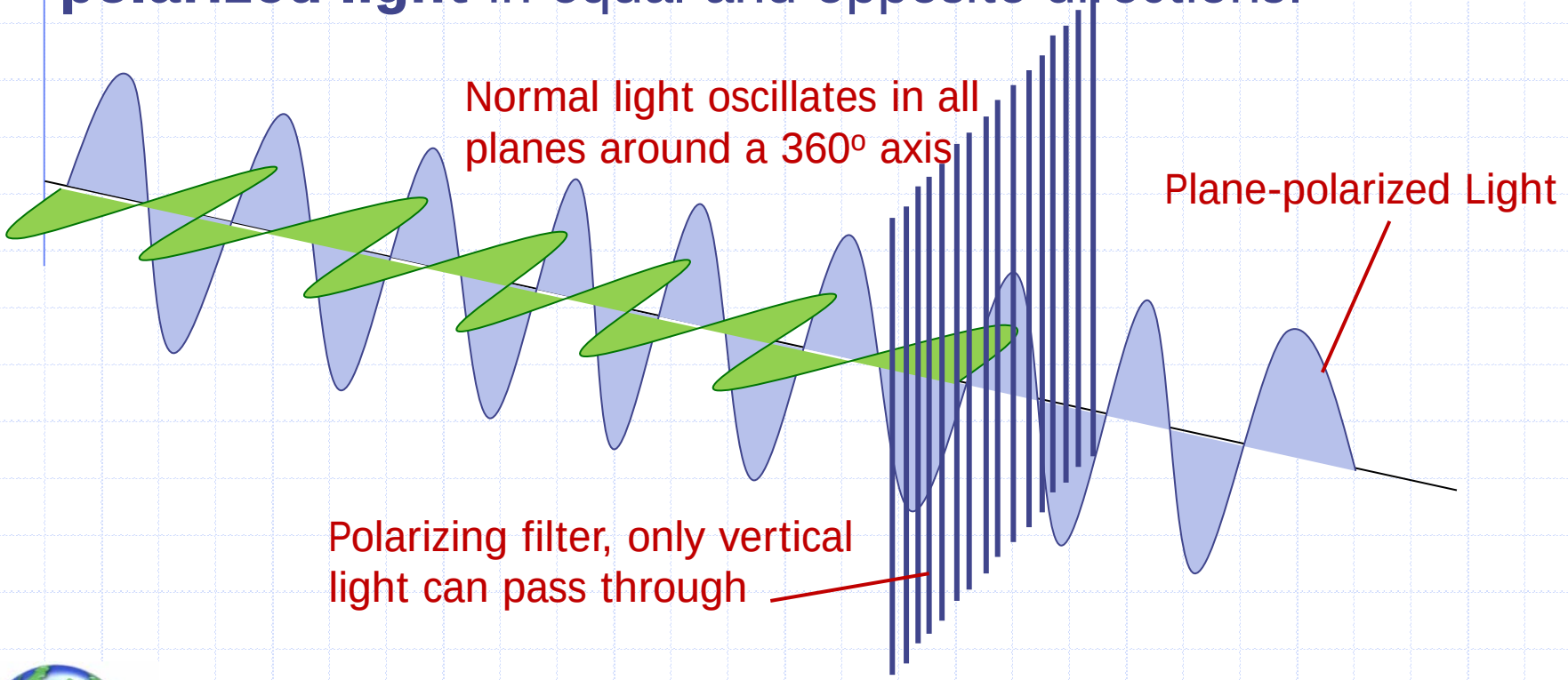
Polarimeter

From Organic Chem (20.6.6)

- The defining method used to distinguish between optical isomers of a compound is to rotate the plane of **plane-polarized light** in equal and opposite directions.



The ability of enantiomers to rotate this plane can be shown using a **polarimeter**

Polarimeter

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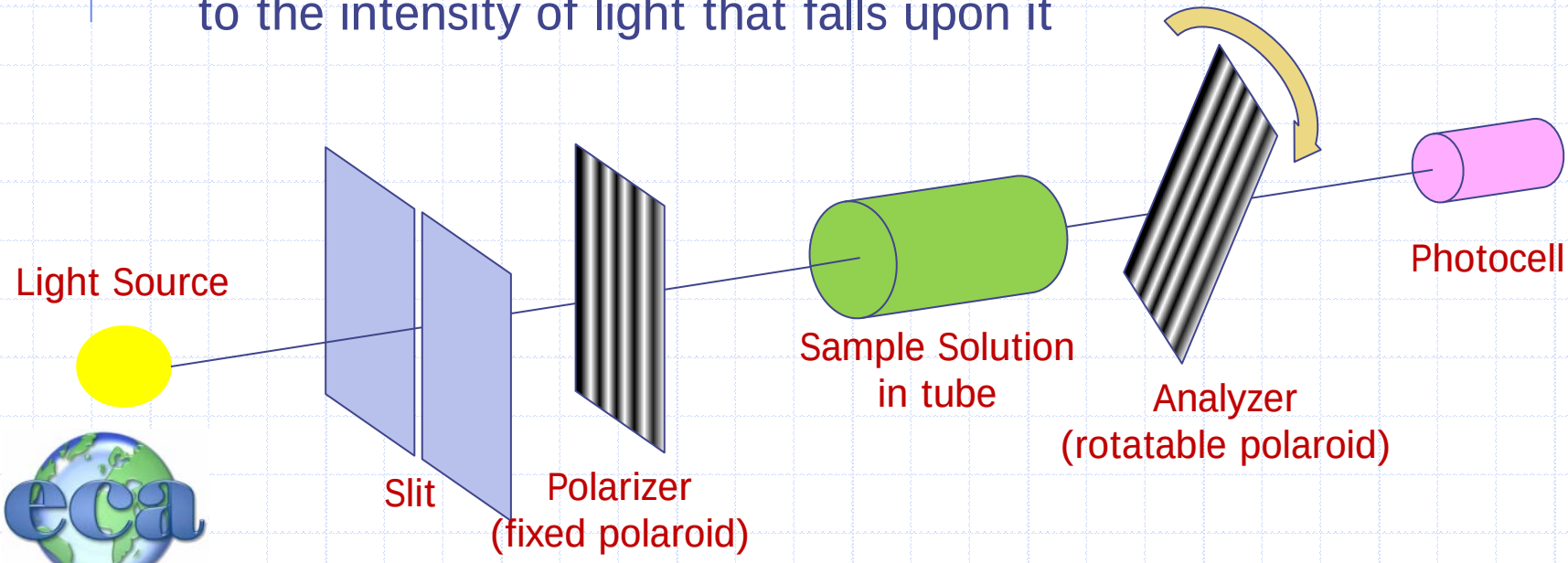
From Organic Chem (20.6.6)

- The **polarimeter** is used to distinguish optical isomers
  - Single wavelength light (monochromatic) passes through a slit to produce a thin beam of light
  - The beam passes through the Polaroid filter
  - Beam passed through sample
  - Beam through another Polaroid (the analyzer)
  - Beam enters the photocell producing an electric current proportional to the intensity of light that falls upon it



Wave Properties

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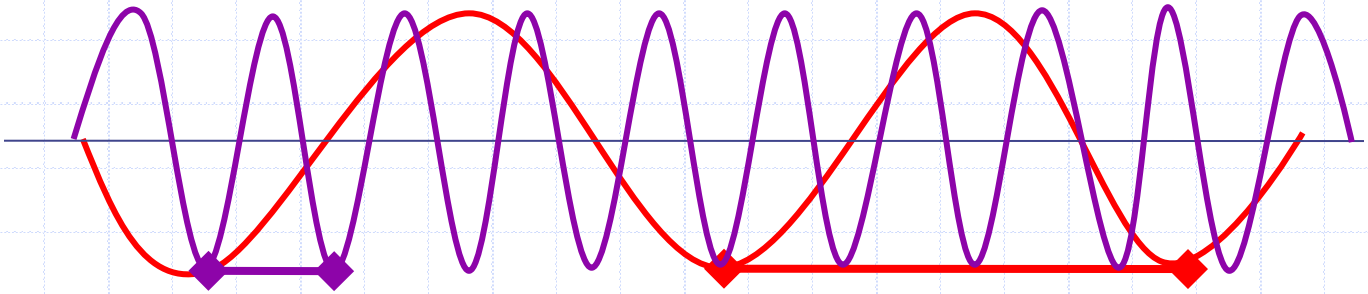
From Atomic Structure (2.3)

- In a vacuum all electromagnetic waves travel at the same speed (c), $c = 3x10^8$ m s^{-1}
- **Wavelength** (lambda, λ) is the distance between two neighboring crests or troughs of a wave
- **Frequency** (*f*) is the number of waves that pass a given point in one second, recorded in **hertz** (Hz)
- **Speed** (c) is the distance travelled by a wave in one second, recorded in meters/second (ms^{-1})
- **Wave Equation** expresses the relationship between each of the three, where c (speed) is the speed of light, $c = 3 \times 10^8$ ms^{-1}.
  - **$C = f\lambda$ or $f = c / \lambda$**



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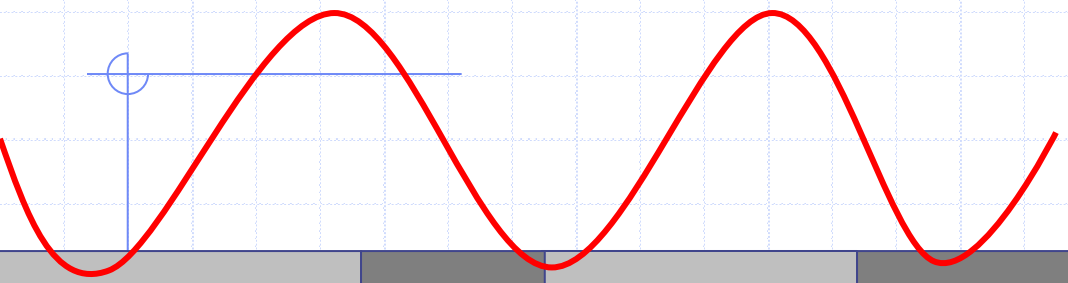
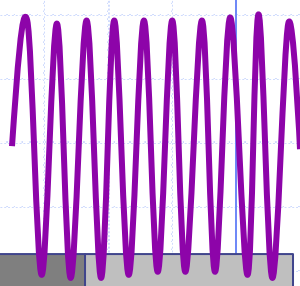
Electromagnetic Spectrum

From Atomic Structure (2.3)





Visible Light

Long-wave Radio	Radio TV	Microwaves (radar)	Infrared		Ultra-violet	X-rays	γ-rays
10^{5} 10^{6} 10^{7}	10^{8} 10^{9}	10^{10} 10^{11}	10^{12} 10^{13} 10^{14}	10^{15}	10^{16} 10^{17}	10^{18}	10^{19}
10^{3} 10^{2} 10 1	10^{-1} 10^{-2}	10^{-3} 10^{-4} 10^{-5}	10^{-6} 10^{-7} 10^{-8}		10^{-9} 10^{-10}	10^{-11}	
10^{-28} 10^{-27} 10^{-26} 10^{-25}	10^{-24} 10^{-23}	10^{-22} 10^{-21} 10^{-20}	10^{-19} 10^{-18} 10^{-17}		10^{-16} 10^{-15}	10^{-14}	

ROYGBIV

Frequency/Hz

Wavelength/m

Energy/J

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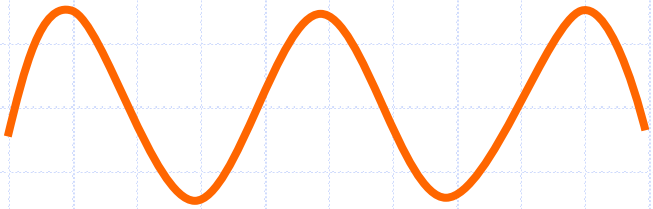
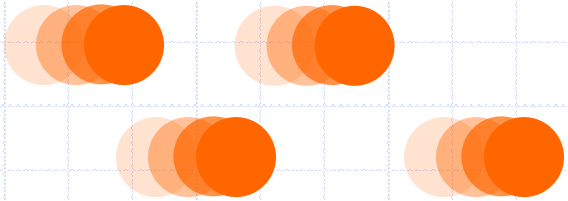
Planck's constant

From Atomic Structure (2.3)

- Light can also be described as particles (photons) which are tiny packets of energy
- The wave and particle models can be related through **Planck's constant**.
  - **$E = hf$**
  - E is the energy of a photon (in joules)
  - h is Planck's constant (6.63×10^{-34} Js)
  - f is the frequency as before





- A Photon of high frequency electromagnetic radiation has more energy than one of low frequency.

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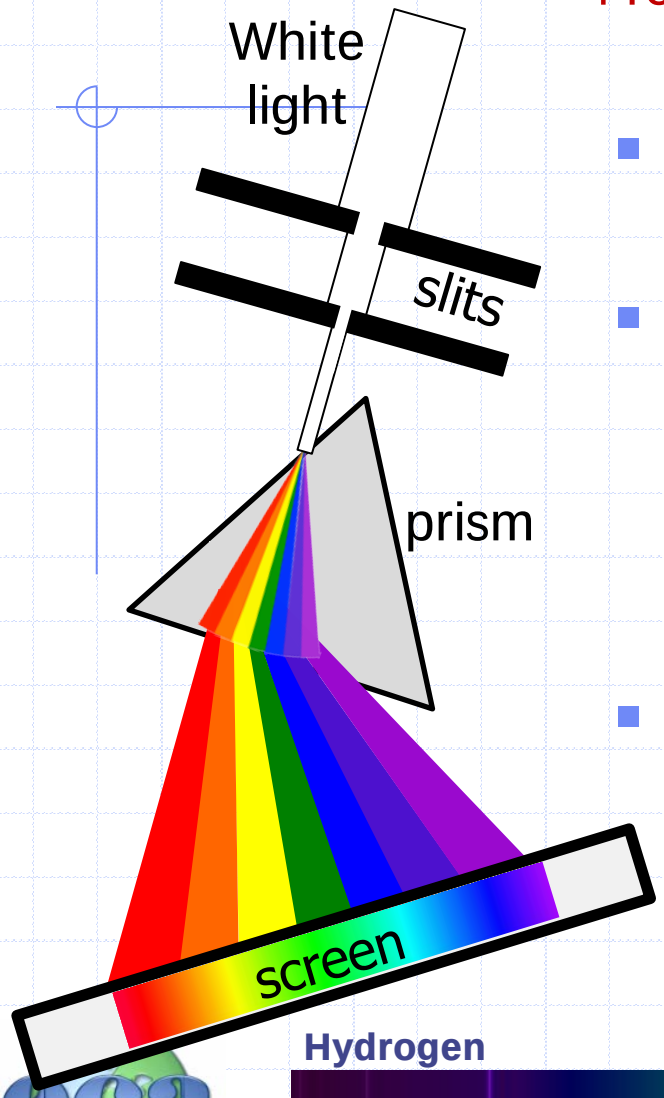
Visible Spectrum (continuous vs line)

From Atomic Structure (2.3)



- **White light** is an intense blend of all colors of light
- A **continuous spectrum** of light is composed of all the visible colors of white light. Like a rainbow where there is a smooth blend of an infinite number of colors
- A **line spectra** is one which contains only a narrow emission of colors on a black background

Hydrogen

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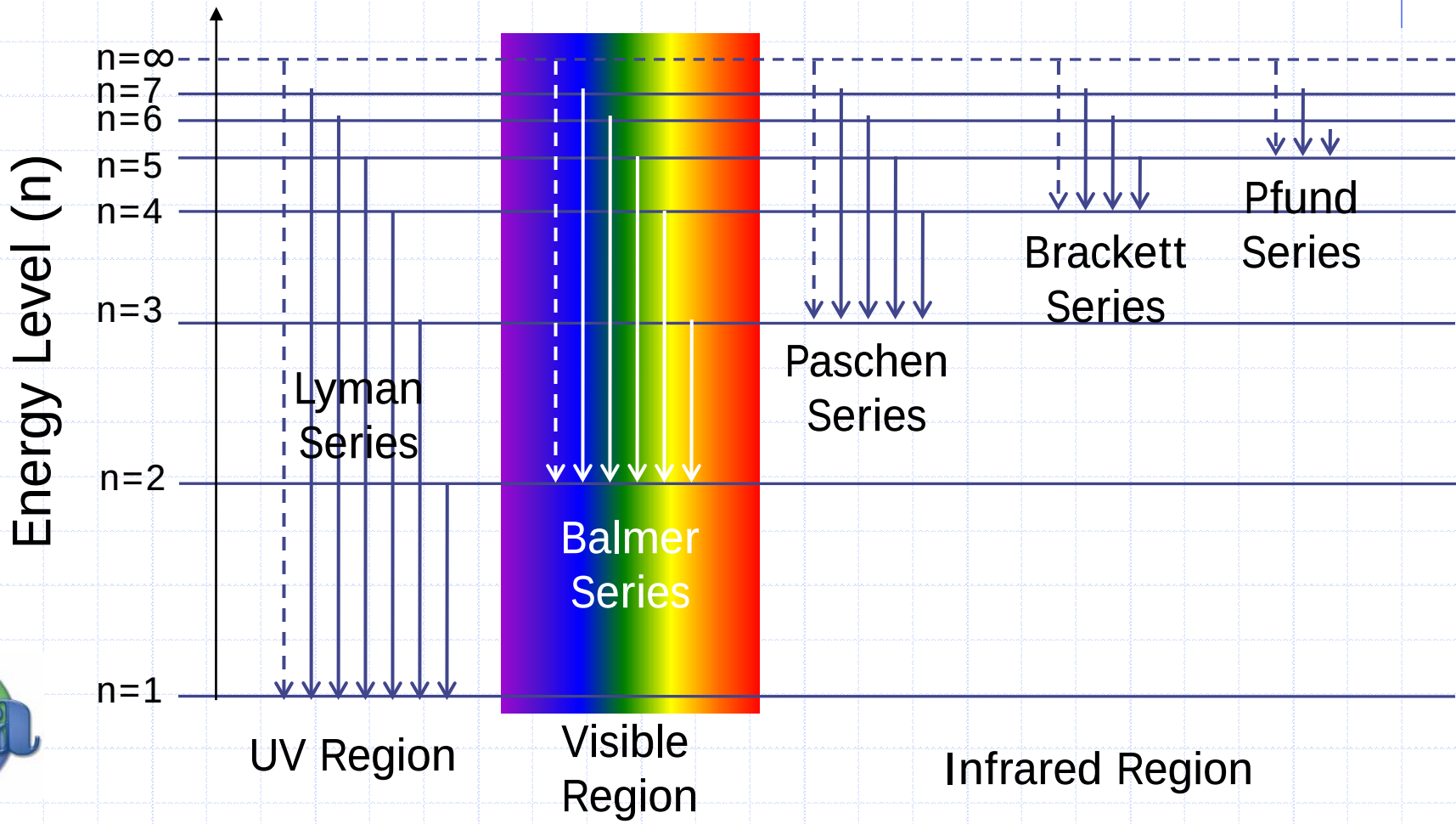
Hydrogen Emission

From Atomic Structure (2.3)

The origin of each of hydrogen's emissions can be summarized through the following diagram



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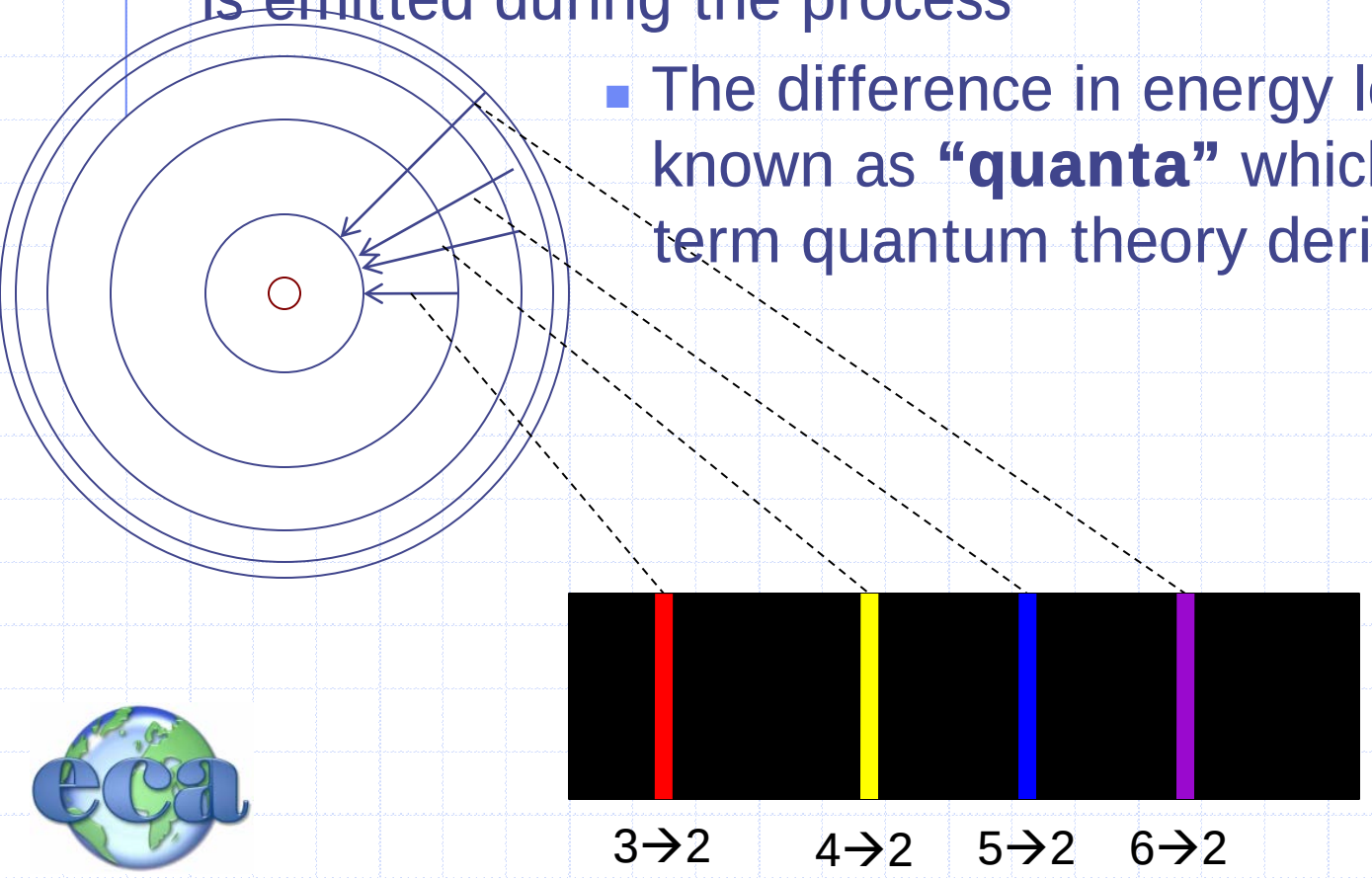
Visible Spectrum Simplified

From Atomic Structure (3.3)

- The difference in energy levels as electrons move corresponds to the energy of the wavelength of light that is emitted during the process
  - The difference in energy level is also known as **“quanta”** which is where the term quantum theory derives itself



**This diagram is an over-simplification of what occurs from level to level. The concept and trend holds true, the specifics about colors do not necessarily*

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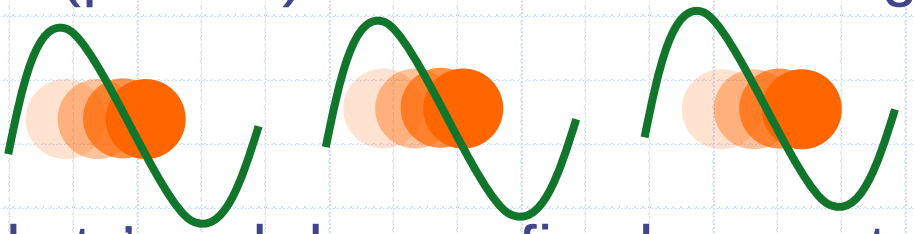
Quantum Theory ‘Packets’

- Since energy does not travel continuously, waves must be cut off at points
- The particle (photon) can be seen as a segment of a wave:



- These ‘packets’ each have a fixed amount of energy (quanta) while makes it useful in investigating atomic and molecular structure

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Waves that carry information

- Communication systems take advantage of the modulation of waves (longitudinal or translational) to carry signals.
- Cell phones, radio signals, etc

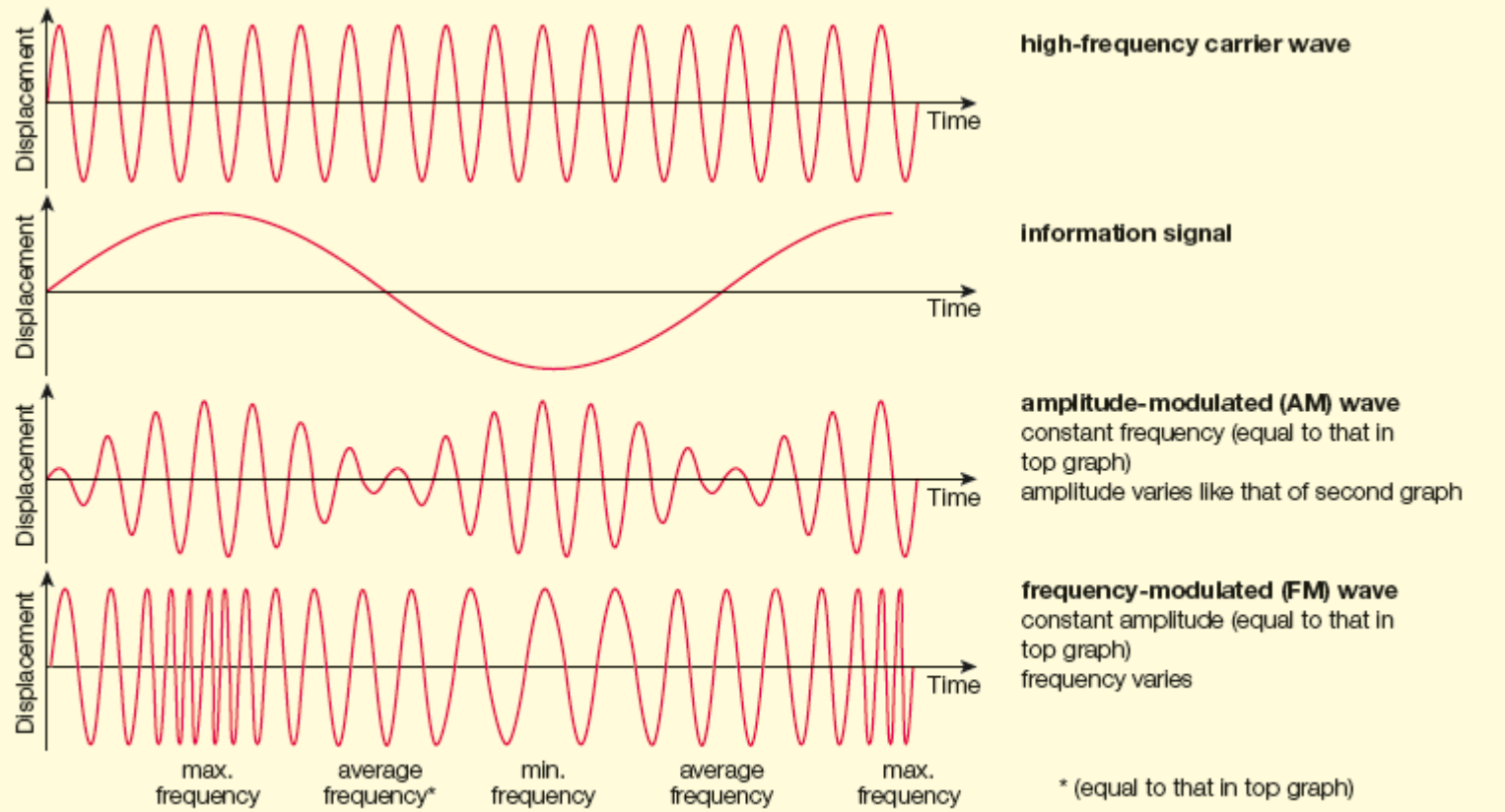

Figure 21.8 Amplitude modulation (AM) and frequency modulation (FM) of a carrier wave

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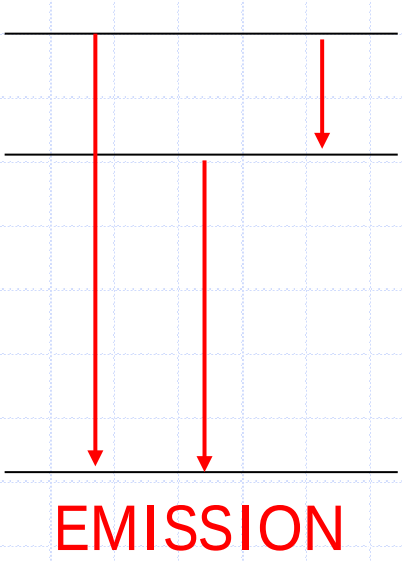
Absorption vs Emission

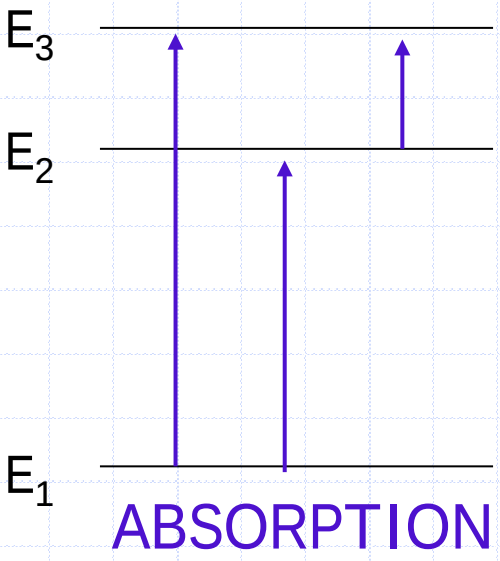
A.2.2 Distinguish between absorption and emission spectra and how each is produced. (2)

- **Emission Spectroscopy**
  - A molecule or atom undergoes a transition from a state of high energy (E_2) to low energy (E_1)
- **Absorption Spectroscopy**
  - A molecule or atom undergoes a transition from a state of low energy (E_1) to high energy (E_2)

The energy emitted or absorbed, which is the frequency (f) of the wave is given by the following relationship:

$$hf = \Delta E = E_2 - E_1$$





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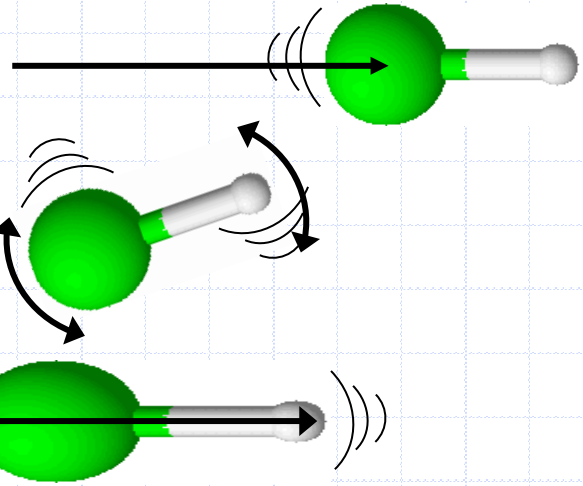
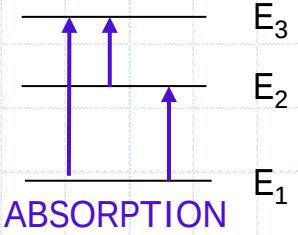
Process of Absorption

A.2.3 Describe the atomic and molecular processes in which absorption of energy takes place. (2)

- Energy is transferred into molecules when they absorb electromagnetic radiation
- This energy can cause a variety of changes to occur in the molecule (the behavior depends on the molecule)
  - **Translation**
    - molecule moving
  - **Rotation**
    - whole or specific bonds rotating
  - **Vibration**
    - stretching
  - **Energy Level Movement**
    - jumps up in energy level





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Relative Energy of Behavior

Large Change in Energy

Electronic Energy (excited state)

Vibrational Energy

Rotational Energy

Small Change in Energy

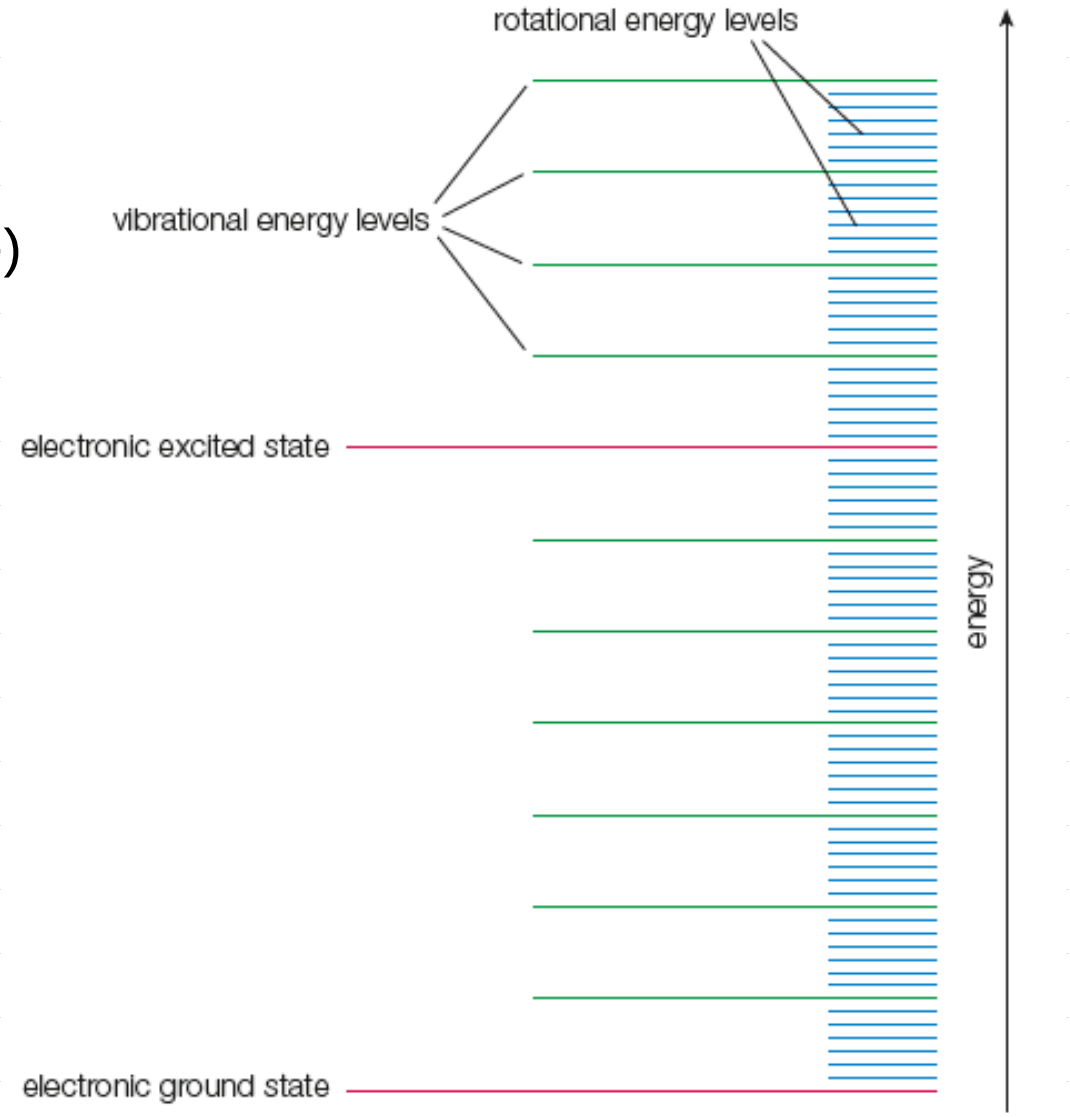

Figure 21.15 The electronic, vibrational and rotational energy levels in a molecule

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Microwaves

Frequency near 3GHz (λ = 10cm)

- Some molecules absorb in the microwave region (just below IR) and result in rotational energy changes
- Water is the perfect example
  - As H_2O absorbs energy it undergoes rotational changes which is converted into translational kinetic energy and temperature rises
  - Plastic and glass containers do not absorb microwaves but metals do!